



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

# The Partnership for Advanced Computing in Europe Research Infrastructure | **PRACE**

## – resources and opportunities

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K. Noga, Ł. Flis, P. Lasoń, M. Magryś, M. Sterzel and Ł. Dutka

*ACC Cyfronet AGH*

Konferencja Użytkowników Komputerów Dużej Mocy – KU KDM'18, 9 march 2018



# PRACE | members

## Hosting Members

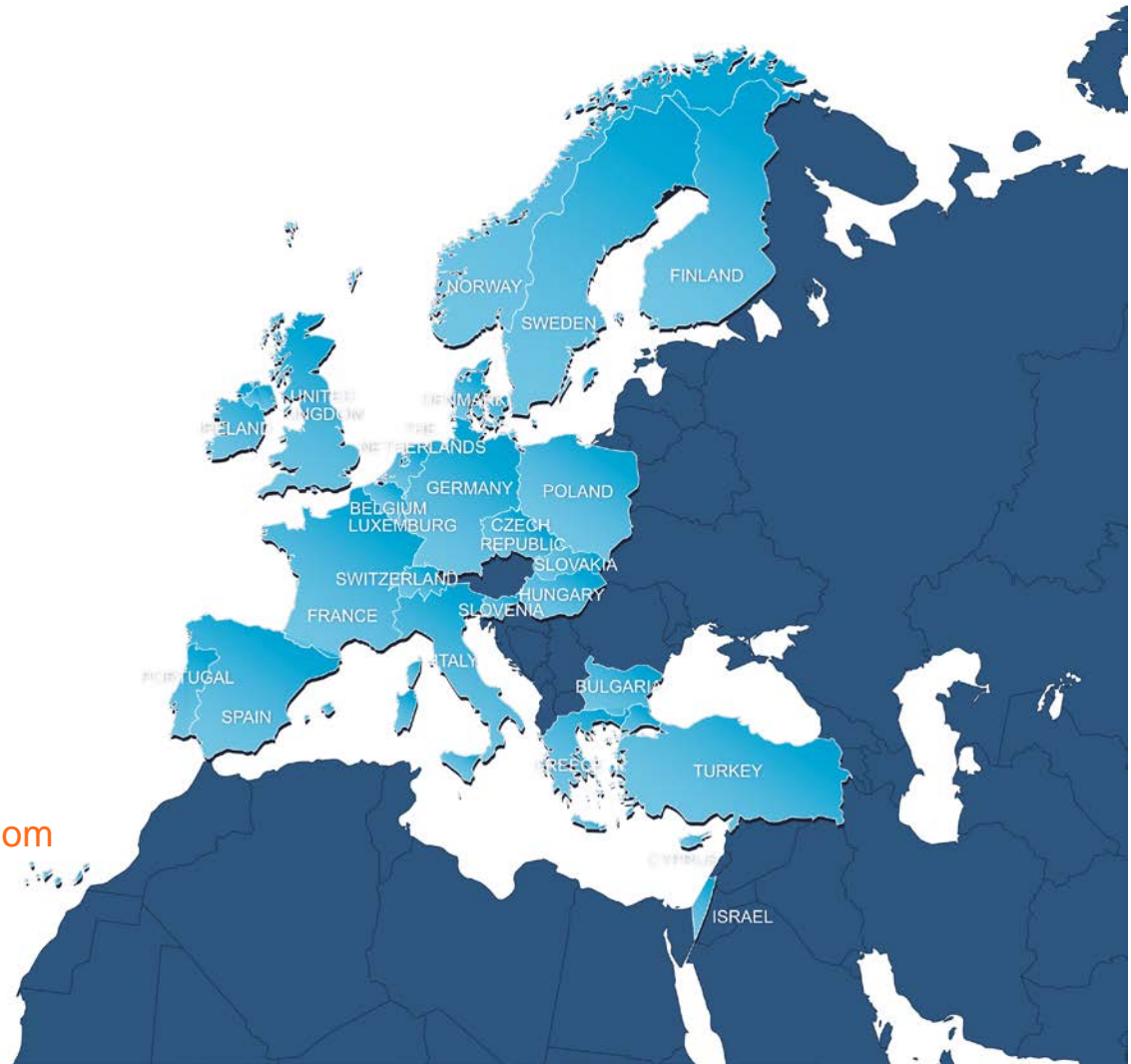
- ▶ France
- ▶ Germany
- ▶ Italy
- ▶ Spain
- ▶ Switzerland

## General Partners (PRACE 2)

- ▶ Belgium
- ▶ Bulgaria
- ▶ Cyprus
- ▶ Czech Republic
- ▶ Denmark
- ▶ Finland
- ▶ Greece
- ▶ Hungary
- ▶ Ireland
- ▶ Israel
- ▶ Luxembourg
- ▶ Netherlands
- ▶ Norway
- ▶ Poland
- ▶ Portugal
- ▶ Slovakia
- ▶ Slovenia
- ▶ Sweden
- ▶ Turkey
- ▶ United Kingdom

## Observers

- ▶ Croatia
- ▶ Romania





## PRACE | what we do

- ▶ **Open access** to world-class HPC systems to EU scientists and researchers
- ▶ **Variety of architectures** to support the different scientific communities
- ▶ High standards in **computational science** and engineering
- ▶ **Peer Review** at European level to foster scientific excellence
- ▶ Robust and persistent **funding scheme** for HPC supported by national governments and European Commission (EC)
- ▶ Support the development of intellectual property rights (**IPR**) in Europe by working with industry and public services
- ▶ Collaborate with European HPC **industrial** users and suppliers



# PRACE | achievements

- ▶ 570 scientific projects enabled
- ▶ 16 000 000 000 (thousand million) core hours awarded since 2010
- ▶ Of which 63% led by another PI nationality than the HM
- ▶ R&D access to industrial users with >50 companies supported
- ▶ >10 000 people trained through PRACE Training
- ▶ >60 Petaflops of peak performance on 7 world-class systems
- ▶ 25 PRACE members, including 5 Hosting Members  
(France, Germany, Italy, Spain and Switzerland)
- ▶ PRACE is the only e-infrastructure Landmark on the ESFRI Roadmap 2016





# PRACE | Tier-0 Systems

**JUQUEEN:** IBM BlueGene/Q  
GAUSS @ FZJ, Jülich, Germany  
#22 Top 500



**MareNostrum:** IBM  
BSC, Barcelona, Spain  
#16 Top 500



**CURIE:** Bull Bullx  
GENCI/CEA, Bruyères-le-Châtel, France  
#93 Top 500

**NEW ENTRY 2016**



**Piz Daint:** Cray XC50  
CSCS, Lugano, Switzerland  
#3 Top 500



**MARCONI:** Lenovo  
CINECA, Bologna, Italy  
#14 Top 500



**SuperMUC:** IBM  
GAUSS @ LRZ, Garching, Germany  
#44 Top 500



**Hazel Hen:** Cray  
GAUSS/HLRS,  
Stuttgart, Germany  
#19 Top 500





# PRACE | project access



**Free-of-charge** required to publish results at the end of the award period



**Preparatory Access** (2 to 6 months)



**Project Access** (12, 24 or 36 months)



**SHAPE Programme** (2 to 6 months)



**Centers of Excellence** : 0,5 % of the total resources available for Centres of Excellence

**Criterion:  
Scientific Excellence  
Assessed by an  
improved review  
process**

[www.prace-ri.eu/call-announcements/](http://www.prace-ri.eu/call-announcements/)



# PRACE | project access



<http://www.prace-ri.eu/prace-project-access/>



# PRACE | project access

- ▶ **17<sup>th</sup> Call for Proposals for Project Access**
  - ▶ Opening of the call: 7 March 2018
  - ▶ Closing of the call: **2 May 2018, 10:00 CET**
  - ▶ Allocation period for awarded proposals: **October 2018 – September 2019**
  - ▶ Type of Access: Project Access and Multi-Year Project Access
- ▶ Applications for Project Access must use codes that have been previously **tested** and
  - ▶ demonstrate **high scalability and optimisation** to multi-core architectures
  - ▶ demonstrate a requirement for ensemble simulations that need a **very large amount of CPU/GPU**





# PRACE | project access

## ▶ 17<sup>th</sup> Call for Proposals for Project Access

System	Architecture	Site (Country)	Core Hours (node hours)	Minimum request
Joliot Curie – SKL	Bull Sequana X1000	GENCI@CEA (FR)	134 million (2.8 million)	15 million core hours
Joliot Curie – KNL	Bull Sequana X1000	GENCI@CEA (FR)	72 million (1.1 million)	15 million core hours
Hazel Hen	Cray XC40 System	GCS@HLRS (DE)	70 million (2.9 million)	35 million core hours
JUWELS	Multicore cluster	GCS@JSC (DE)	70 million (1.5 million)	35 million core hours
Marconi-Broadwell	Lenovo System	CINECA (IT)	36 million (1 million)	15 million core hours
Marconi-KNL	Lenovo System	CINECA (IT)	612 million (9 million)	30 million core hours
MareNostrum	Lenovo System	BSC (ES)	240 million (5 million)	15 million core hours
Piz Daint	Cray XC50 System	CSCS (CH)	510 million (7.5 million)	68 million core hours Use of GPUs
SuperMUC SuperMUC-NG	Lenovo NextScale/ Lenovo ThinkSystem	GCS@LRZ (DE)	105 milion (3.8 million)	35 million core hours



# PRACE | project access

## ▶ 18<sup>th</sup> Call

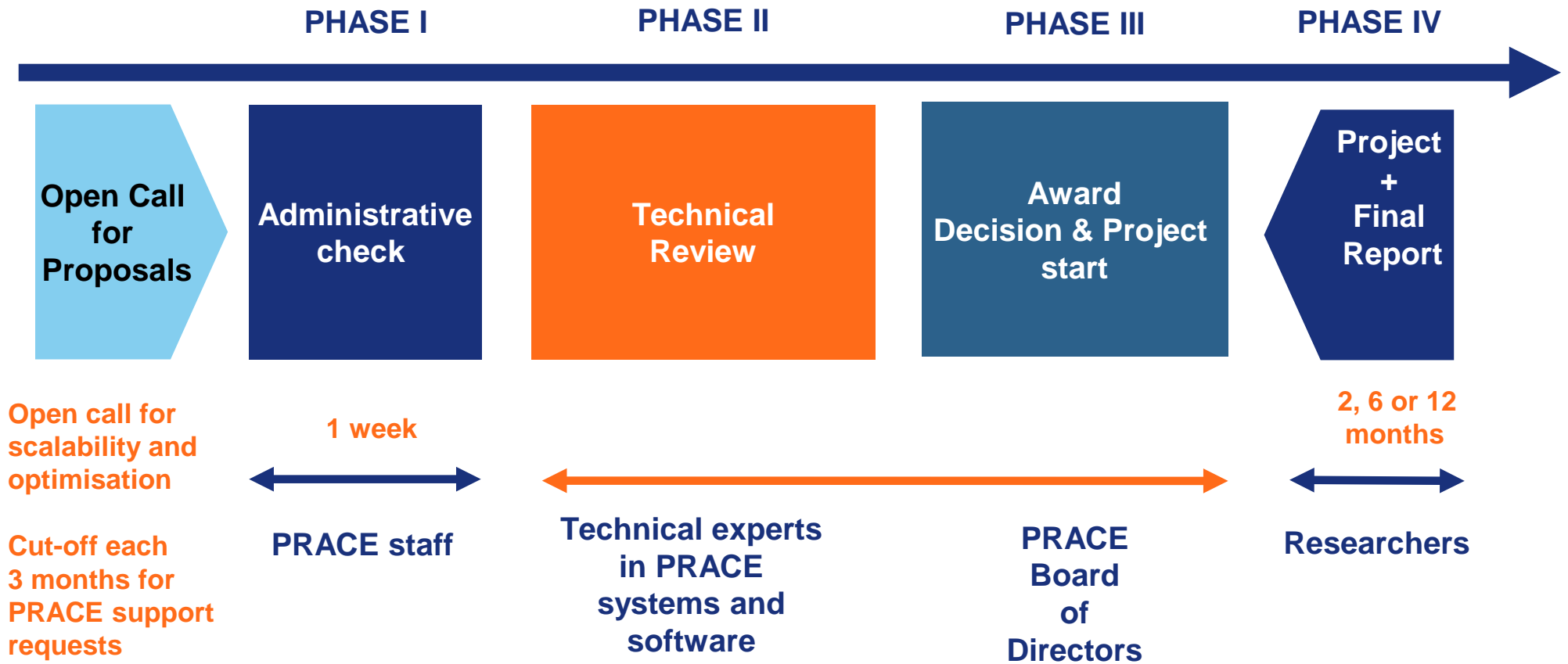
- ▶ Opening of the call: 4 September 2018
- ▶ Closing of the call: 30 October 2018, 10:00 CET
- ▶ Allocation period: From 2 April 2019 to 1 April 2020

## ▶ 19<sup>th</sup> Call

- ▶ Opening of the call: 5 March 2019
- ▶ Closing of the call: 30 April 2019, 10:00 CEST
- ▶ Allocation period: From 1 October 2019 to 30 September 2020



# PRACE | preparatory access



<http://www.prace-ri.eu/prace-preparatory-access/>



# PRACE | preparatory access

- ▶ **Open call for scalability and optimisation**
  - ▶ To allow users to optimise, scale and test codes on PRACE Tier-0 systems before applying to PRACE calls for Project Access
  - ▶ Type A - performance and scalability tests (up to 2 months)
  - ▶ Type B - code development and optimisation (up to 6 months)
  - ▶ Type C - code development and optimisation with PRACE experts support (up to 6 months and 6 PM)
  - ▶ Type D - code adaption and optimisation process on a PRACE Tier-1 system with PRACE experts support (up to 12 months and 6 PM)
    - ▶ towards the end of the project Tier-0 computing time (in form of the Type A scheme) to test the scalability improvements
- ▶ **Cut-off each 3 months for PRACE support requests**
  - ▶ 1 July 2018, 11:00 CEST – 33<sup>rd</sup> cut-off for Type C and Type D





# PRACE | Training and Outreach activities

provide a sustained, high-quality training and education service for the European HPC community



6 PRACE Advanced Training Centres (PATCs) and 4 Training Centres (PTCs)



PRACE training events: Seasonal Schools, International HPC Summer School, On-demand training events



Summer of HPC (programme for undergraduate and postgraduate students)



PRACE Training and Events portal



CodeVault, Massive Open Online Courses (MOOCs)

## Training topics

Different levels of training

- ▶ Basic, intermediate, advance

High performance computing

- ▶ Parallel programming
- ▶ Accelerators
- ▶ Performance optimization

Domain-specific topics

- ▶ Simulation software
- ▶ Visualization
- ▶ Data intensive computing



# PRACE | Training and Events Portal

- ▶ [www.training.prace-ri.eu](http://www.training.prace-ri.eu)
- ▶ Single hub for the PRACE training events, training material and tutorials
- ▶ PATC Programme 2017-2018
  - ▶ 79 courses, 215 training days
  - ▶ New courses on forward-looking topics
  - ▶ New hardware and programming paradigms
  - ▶ Data science
  - ▶ Collaboration with CoEs on several courses

## Tentative PATC and PTC Training Programme: March 2018 to July 2018

### March 2018

- Introduction to simulation environments for Life sciences (BSC)
- Python for computational science (CINECA)
- Programming paradigms for GPU devices (CINECA)
- Advanced Fortran Programming (CSC)
- Spring School in Computational Chemistry (CSC)
- HPC Tools Workshop (EPCC)
- Object-Oriented programming for HPC (EPCC)
- Parallel I/O and Portable Data Formats (GCS)
- OpenMP GPU Directives for Parallel Accelerated Supercomputers (GCS)
- Parallel Programming with HPX (GCS)
- Data Management Plan – Long term preservation (MdS)
- Runtime systems for heterogeneous platform programming (MdS)
  - Parallel programming with MPI/OpenMP (SURFsara)

### April 2018

- Programming of Petaflop Machine (BSC)
- High Performance Molecular Dynamics (CINECA)
- Advanced Threading and Optimisation (CSC)
- Data Carpentry (EPCC)
- VI-HPS Tuning Workshop (GCS)
- Advanced Topics in HPC (GCS)
- Advanced Fortran for Scientific Computing (GCS)
- GPU Programming with CUDA (GCS)
- Parallel linear algebra (MdS)
  - Introduction to biomolecular modelling and molecular dynamics in HPC (GRNET)
  - Advanced topics in HPC programming (SURFsara)

- Advanced Usage on CURIE: parallelism, optimization, IO, tools (MdS)
- Uncertainty quantification (MdS)
- Introduction to PETSc (MdS)
  - Accelerator programming (GPU programming using CUDA and OpenACC) (GRNET)
  - Many-core programming and performance profiling for molecular and atomic simulations (ICHEC)
  - PETSc tutorial (IT4I)

### June 2018

- Introduction to programming in CUDA (BSC)
- 4th School On Scientific Data Analytics and Visualization (CINECA)
- High-Throughput on High-Performance and Cloud Computing with AiiDA (CINECA)
- Efficient Parallel IO (EPCC)
- Introduction to Unified Parallel C (UPC) and Co-Array Fortran (CAF) (GCS)
- Efficient parallel Programming with GASPI (GCS)
- High-Performance Computing with Python (GCS)
- Intel MIC / Knights Landing Programming Workshop (GCS)
- Node-Level Performance Engineering (GCS)
- High-performance scientific computing in C++ (GCS)
  - HPC & Data Analytics (GCS)
  - Meteorological and climate modelling (GRNET)
  - Efficient data formats and Streaming data processing in the Apache Big Data ecosystem (SURFsara)

### July 2018

- PUMPS (BSC)
- Message-Passing Programming with MPI (EPCC)



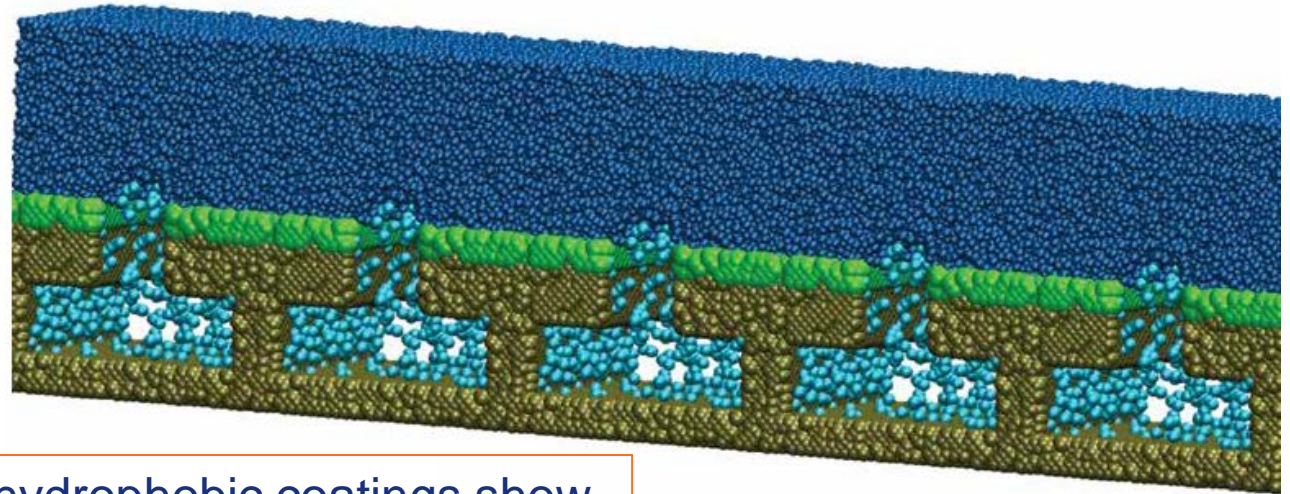
# Superhydrophobic coatings inspired by nature

## Facts & Figures

Alberto Giacomello,  
Sapienza University of  
Rome

**SLIP- Salvinia –  
inspired surfaces in  
action: slip, cavitation,  
and drag reduction**

Awarded **50 million core  
hours** on FERMI hosted  
at CINECA, Italy



Superhydrophobic coatings show great promise for underwater applications.

Focused on this goal - the **SLIP project** has studied a new generation of superhydrophobic coatings based on the structure of the floating fern Salvinia.



## IMAGINE\_IT project – Greater understanding of earthquakes

### Facts & Figures

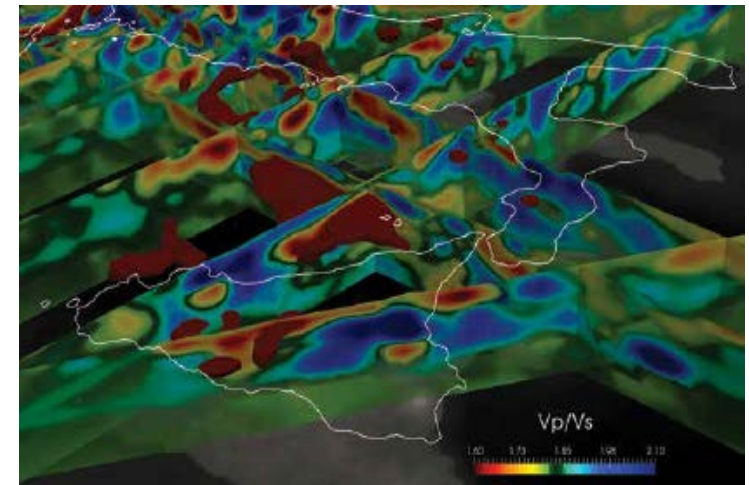
Dimitri Komatitsch,  
CNRS, France,  
Emanuele Casarotti,  
INGV, Italy

**IMAGINE\_IT - 3D full-wave tomographic IMAGING of the Entire Italian lithosphere**

Awarded **40 million core hours** on Curie hosted by GENCI at CEA, France

Protecting society from the effects of earthquakes is crucial societal goal.

Focused on this goal - the **IMAGINE\_IT project** has developed a model of the lithosphere below the entirety of Italy based on highly accurate seismic wave imaging.



*Three-dimensional view from SSW of the seismic velocity structure beneath the Tyrrhenian magmatic province.*



## SMOC project – ocean modelling for Climate Research

### Facts & Figures

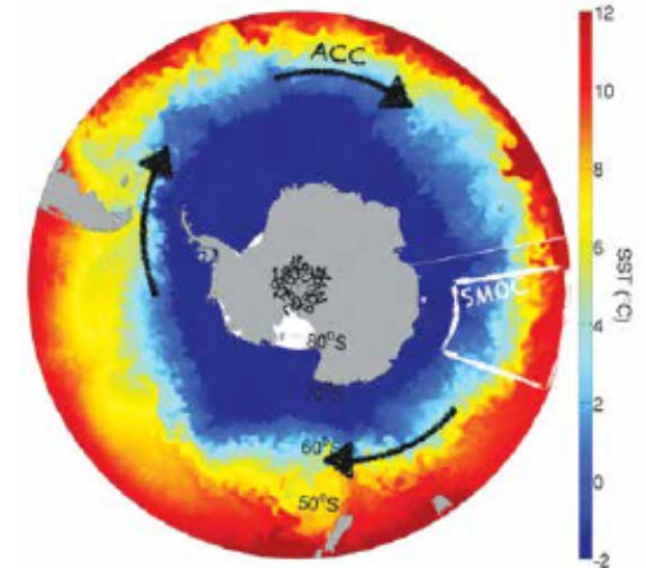
Xavier Capet, CNRS,  
France

### SMOC - Submesoscale ocean Modeling for Climate

Awarded **11 million  
core hours** on HERMIT  
hosted by **GCS** at  
**HLRS, Germany**

The ocean is a hugely complex system and has crucial impact on the earth climate. Understanding how it works is a fundamental scientific challenge.

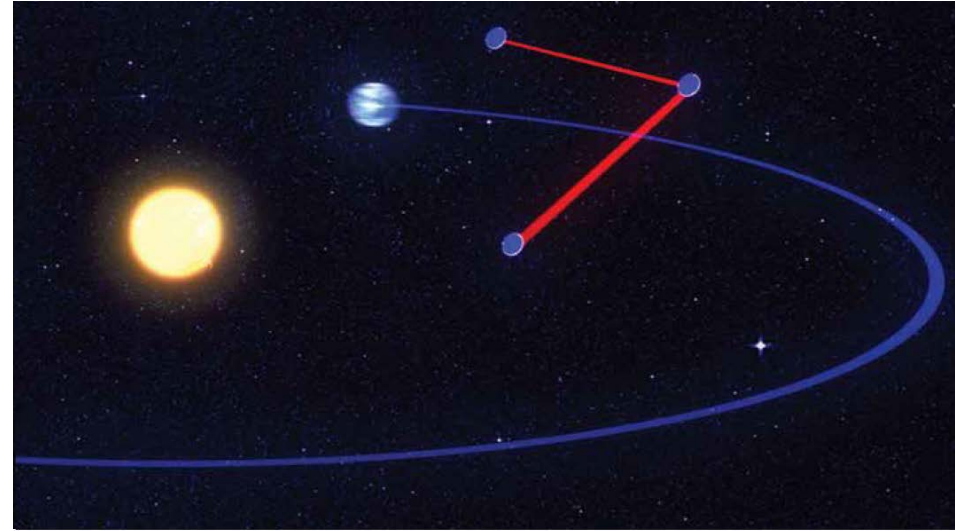
The **results of SMOC** will be used to inform climate systems about what they are missing and thus **improve climate predictions.**



*Polar view of the sea surface temperature as simulated by a global ocean model. The Antarctic continent is surrounded by cold waters with progressively warmer water at lower latitude (toward the outer edge of the image).*

## Gravitational waves from the early universe

Simulations of violent events following the Big Bang that may have produced gravitational waves under study generates huge amounts of data used to determine what cosmological processes could be detected and which mission design represents the best prospects for scientific discovery. The results of this work provide a basis for understanding what the waves can tell us about the universe and physics beyond the Standard Model.



The three LISA spacecraft will be placed in orbits that form a triangular formation with centre  $20^\circ$  behind the Earth and side length 1 million km (the figure showing the formation is not to scale.) Each spacecraft will be in an individual Earth-like orbit around the Sun.



*What we have achieved on the supercomputing resources provided by PRACE is at the very limit of our technological capabilities today.*

- ▶ David J. Weir, University of Helsinki, Finland
- ▶ Resources awarded: 17.6 million core hours on Hazel Hen hosted by GCS at HLRS





PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

# HPC for Innovation: when Science meets Industry

<http://www.prace-ri.eu/pracedays18/>



Scientific and  
Industrial  
Conference 2018



SAVE THE DATE!  
29 – 31 May 2018

HPC for Innovation:  
when **Science**  
meets **Industry**

Univerza v Ljubljani

LJUBLJANA,  
SLOVENIA



European HPC Summit Week  
28 May to 1 June 2018  
Ljubljana



Photo: Tomo Jeseničnik



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

# THANK YOU FOR YOUR ATTENTION

[www.prace-ri.eu](http://www.prace-ri.eu)



Ministry of Science  
and Higher Education  
Republic of Poland

**"Prace realizowane przy wsparciu Ministerstwa Nauki i Szkolnictwa Wyższego,  
decyzja nr DIR/WK/2016/18"**





**Criterion:  
Scientific  
Excellence**

# PRACE | SHAPE

- ▶ SME HPC Adoption Programme in Europe
  - ▶ Equip European SMEs with expertise to take advantage of the innovation possibilities of HPC
  - ▶ Increasing competitiveness
  - ▶ Enable development of new products or services
  - ▶ Create new business opportunities

